2-Methylmercaptomethyl-2-butenal

Inchi: InChI=1S/C6H10OS/c1-3-6(4-7)5-8-2/h3-4H,5H2,1-2H3/b6-3-
InchiKey: IBSLHWQWKUNIJE-UTCJRWHESA-N
Formula: C6H10OS
SMILES: CC=C(C=O)CSC
Mol. weight [g/mol]: 130.21

Physical Properties

Property code	Value	Unit	Source
gf	4.91	kJ/mol	Joback Method
hf	-103.45	kJ/mol	Joback Method
hfus	16.61	kJ/mol	Joback Method
hvap	42.53	kJ/mol	Joback Method
log10ws	-1.35		Crippen Method
logp	1.495		Crippen Method
mcvol	109.020	ml/mol	McGowan Method
pc	3690.97	kPa	Joback Method
ripol	1713.00		NIST Webbook
ripol	1713.00		NIST Webbook
tb	458.16	K	Joback Method
tc	667.40	K	Joback Method
tf	214.74	K	Joback Method
vc	0.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	208.32	J/mol×K	458.16	Joback Method
cpg	218.50	J/mol×K	493.03	Joback Method
cpg	228.13	J/mol×K	527.91	Joback Method
cpg	237.24	J/mol×K	562.78	Joback Method
cpg	245.85	J/mol×K	597.65	Joback Method
cpg	253.98	J/mol×K	632.53	Joback Method
cpg	261.64	J/mol×K	667.40	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R640872&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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